Benzeneacetic acid, 4-hydroxy-156-38-7 | DTXSID5059745

156-38-7	DTXSID5059745	

Model Performance

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Model	II)ata
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Weighted KNN model

5-fold CV ((75%)	Training (75%)		Test (25%	Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE	
0.95	0.69	0.95	0.65	0.96	0.68	

Model Results

Predicted value: 7.84

Global applicability domain: Outside

Local applicability domain index: 2.55e-01

Confidence level: 4.22e-01

Nearest Neighbors from the Training Set

Image not found

4-Hydroxybenzoic acid

Measured: 8.08 Predicted: 7.78

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Salicylic acid

Measured: 7.44 Predicted: 7.60

Image not found

Methylparaben

Measured: 8.57 Predicted: 7.06

Image not found

1-Octanol

Measured: 6.03 Predicted: 5.95 Image not found

Phenacetin
Measured: 9.59
Predicted: 9.23